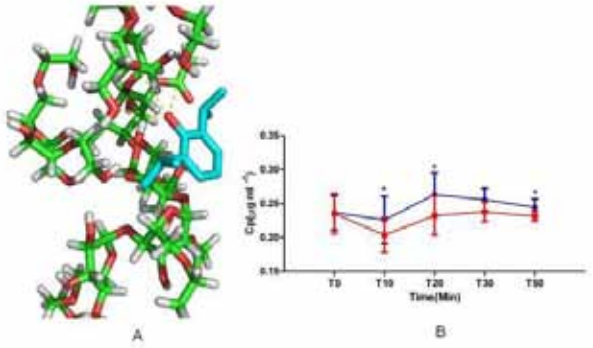
Results and Discussion: Docking studies: the predicted free energy for HES-propofol complexes was negative, -3.6 kJ.mol^{-1} (best ranking pose)



[Figure 1. A) Representation the best conformation for the connection between propofol and HES. B) Propofol concentrations measured in the two groups of samples (blue line - lactated Ringer's and human plasma) and red line (Hydroxyethyl starch 140/0.3 and human plasma). Mean and standard deviation of the concentrations at the different sampling time points (T0-T50 are shown.]

which favors the propofol-HES interaction and is strengthened by the values of free energy of -2.4 kJ.mol^{-1} obtained for the controls. The laboratorial study showed significant differences through time (p=0.032) and significantly lower propofol in the HES than LR (p=0.019), Fig1B. Shift variations in the IR and ^{1}HNMR spectra of the mixture provided evidence for the formation of inclusion complexes in solution.

Conclusion: Propofol is predicted as being able of establishing hydrogen interactions with the hydroxyl groups of the glucose units of HES which should be further investigated and considered in clinical situations where both drugs are used.

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Acknowledgements: COMPETE: FCOMP-01-0124-FEDER-009525, (PTDC/CVT/101999/2008), SFRH/BPD/75697/2011, PestC/EQB/LA0006/2011, CEQUIMED - PEst-OE/SAU/UI4040/2011.

9AP5-4

A nomogram to calculate estimated glomerular filtration rate (eGFR)

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Background and Goal of Study: eGFR provides a measure of renal function, and is usually calculated using the MDRD equation[1]. This is difficult to calculate without a calculator or computer, and un-noticed key-stroke errors may occur, giving erroneous results.

We have developed a nomogram which carries out the calculation rapidly to a high degree of accuracy. All data are constrained to appropriate clinical ranges; accuracy is greater at lower creatinine levels through use of logarithmic scales; and calculations may be readily perfomed in reverse to check for data entry error. Our nomogram also includes details of Chronic Kidney Disease (CKD) grading, and advice on the use of Non Steroidal Anti-Inflammatory Drugs in renally impaired patients[2].

Materials and Methods: The nomogram was created using standard techniques, and drafted in Pynomo, an open-source software package. A spreadsheet (Excel, Microsoft Corp, WA) was used to randomly generate 100 sets of simulated values for gender, age and creatinine level. The eGFR was then calculated in each case using both the nomogram and Excel; and Bland-Altman (BA) analysis was performed[3].

Results and Discussion: The BA plot (Fig 2) showed very close agreement between spreadsheet and nomogram. Bias of the nomogram was -0.13mL/min/1.73m^2, with limits of agreement -0.8 to 0.6mL/min/1.73m^2.

Conclusion(s): Our nomogram provides a low cost rapid method for calculation of eGFR to a clinically acceptable level of accuracy. It is a prescribing aid for healthcare professionals; and may be used to check calculations performed by other means; or as an alternative if these are not available.

References:

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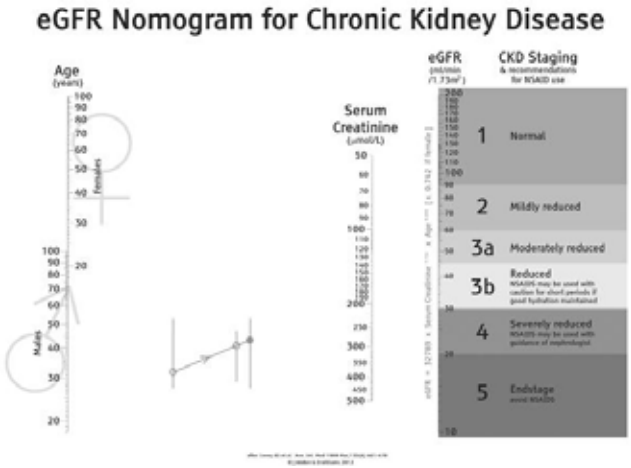
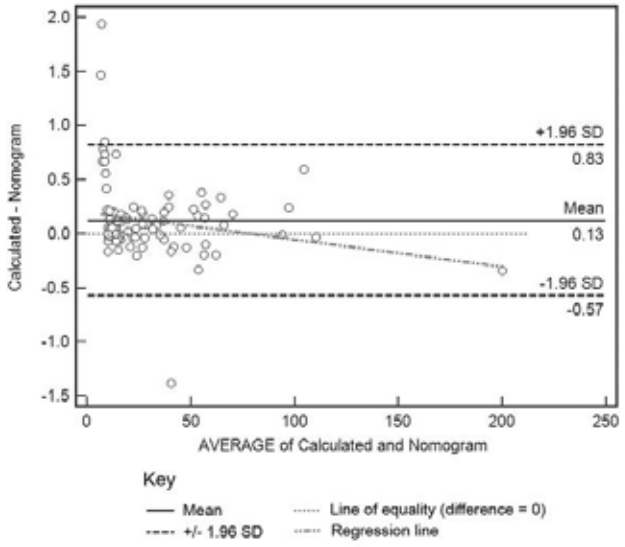


[Fig 1. The eGFR Nomogram]



[Fig 2. Bland-Altman plot]

9AP5-5

Influence of heparin on mediators of inflammation

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Background and Goal of Study: Surgical trauma leads to stress-response [1]. Overproduction of cytokines increases the risk of organ failure [2]. Heparin can probably reduce the symptoms of inflammation and improve outcomes [3].

The Goal: To study the effects of heparin on mediators of inflammation after selective abdominal surgery.

Materials and Methods: After local ethics committee approval and obtaining informed consent, 50 patients were prospectively divided into two groups depending on the type of thromboprophylaxis. Non-fractioned heparin (NFH) was used in group 1 (n=26): 5000 U 2 hours before surgery and 5000 U twice a day during 7 days after surgery. Bemiparin was used in group 2 (n=24): 2500 U 2 hours before surgery and 2500 U once a day during 7 days after surgery. The patients were comparable according to sex, age, concomitant pathology, ASA class (I-II), type of surgery (laparoscopic cholecistectomy, hernioplasty) and type of anesthesia (total intravenous anesthesia with relaxation).